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TO: Cybille Delacroix
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Wednesday, June 23, 2004
Art Unit: 1614
Phone: 272-0572
Serial Number: 10 / 038114

From: Jan Delaval
Location: Biotech-Chem Library
Rem 1A51
Phone: 272-2504

jan.delaval@uspto.gov

Search Notes

10/038,114

FILE 'USPATFULL' ENTERED AT 17:00:29 ON 23 JUN 2004
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FILE 'HCAPLUS' ENTERED AT 17:00:29 ON 23 JUN 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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FILE 'HCAOLD' ENTERED AT 17:00:29 ON 23 JUN 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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=> s l3 and (?glaucom? or ocular? or intra(2a)ocular? or ophthal? or eye or
intraocular?)
L4 5 L3 AND (?GLAUCOM? OR OCULAR? OR INTRA(2A) OCULAR? OR OPHTHAL?
OR EYE OR INTRAOCULAR?)

=> dup rem l5
L5 IS NOT VALID HERE
The L-number entered has not been defined in this session, or it
has been deleted. To see the L-numbers currently defined in this
session, enter DISPLAY HISTORY at an arrow prompt (=>).

=> dup rem l4
DUPLICATE IS NOT AVAILABLE IN 'HCAOLD'.
ANSWERS FROM THESE FILES WILL BE CONSIDERED UNIQUE
PROCESSING COMPLETED FOR L4
L5 5 DUP REM L4 (0 DUPLICATES REMOVED)

=> d l5 abs ibib kwic hitstr 1-5

L5 ANSWER 1 OF 5 USPATFULL on STN
AB Provided is a method of treating or ameliorating certain fibrotic
diseases or other indications in an animal, including a human,
comprising administering an effective amount of a compound of the
formula I:

Y--Ar.sup..sym..X.sup.-

wherein Ar.sup..sym. is heteroaryl with a quaternary nitrogen, Y defines
certain substitutions on the quaternary nitrogen, and X.sup.- is anion.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

ACCESSION NUMBER: 2004:127511 USPATFULL
TITLE: Method for treating fibrotic diseases or other
indications IIIC
INVENTOR(S): Wagle, Dilip, New York, NY, UNITED STATES
Gall, Martin, Morristown, NJ, UNITED STATES
Bell, Stanley C., Narberth, PA, UNITED STATES
LaVoie, Edmond J., Princeton Junction, NJ, UNITED
STATES

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 2004097495	A1	20040520

DELACROIX

APPLICATION INFO.: US 2003-691839 A1 20031023 (10)
 RELATED APPLN. INFO.: Continuation of Ser. No. US 2001-36857, filed on 31 Dec
 2001, PENDING

	NUMBER	DATE
PRIORITY INFORMATION:	US 2000-259294P	20001229 (60)
	US 2001-259238P	20010102 (60)
	US 2001-296246P	20010606 (60)
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	APPLICATION	
LEGAL REPRESENTATIVE:	MINTZ, LEVIN, COHN, FERRIS, GLOVSKY, AND POPEO, P.C., ONE FINANCIAL CENTER, BOSTON, MA, 02111	
NUMBER OF CLAIMS:	49	
EXEMPLARY CLAIM:	1	
LINE COUNT:	3287	

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

SUMM [0106] The effect of diabetes on the **eye** is called diabetic retinopathy and involves changes to the circulatory system of the retina. The earliest phase of the disease. . . phases of the disease, continued abnormal vessel growth and scar tissue may cause serious problems such as retinal detachment and **glaucoma**. First agents are used to treat, prevent, reduce or ameliorate diabetic retinopathy. The agents can be administered by the methods described below, including by topical administration to the **eye**. The agents can also be administered by intravitreal implant.

SUMM [0123] Pharmaceutical compositions of the invention include administering an **intraocular** pressure decreasing amount of a compound of the formula I.

SUMM [0325] Compositions can also be used to deliver the compound to the site where activity is desired; such as **eye** drops, gels and creams for **ocular** disorders.

SUMM . . . compositions of this invention include aqueous solutions comprising a safe and effective amount of a subject compound intended for topical **intraocular** administration. Such compositions preferably comprise from about 0.01% to about 0.8% w/v of a subject compound, more preferably from about. . .

SUMM [0330] The compounds of the invention are administered by **ocular**, oral, parenteral, including, for example, using formulations suitable as **eye** drops. For **ocular** administration, ointments or droppable liquids may be delivered by **ocular** delivery systems known to the art such as applicators or **eye** droppers. Such compositions can include mucomimetics such as hyaluronic acid, chondroitin sulfate, hydroxypropyl methylcellulose or polyvinyl alcohol, preservatives such as. . .

IT 13076-43-2P 63828-55-7P **454704-85-9P 454704-86-0P**
454704-87-1P 454704-88-2P 454704-89-3P 454704-90-6P
 454704-91-7P

(preparation of thiadiazolium, pyridinium and pyrimidinium salts for treating fibrotic diseases)

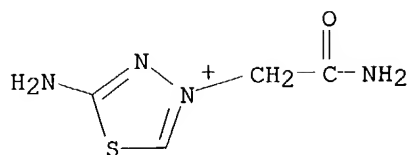
IT **454704-85-9P 454704-86-0P 454704-87-1P**

(preparation of thiadiazolium, pyridinium and pyrimidinium salts for treating fibrotic diseases)

RN 454704-85-9 USPATFULL

CN 1,3,4-Thiadiazolium, 5-amino-3-(2-amino-2-oxoethyl)-, bromide (9CI) (CA
 INDEX NAME)

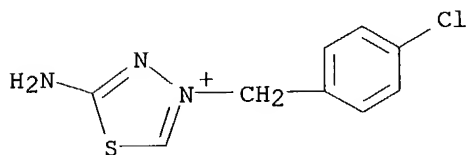
10/038,114



● Br⁻

RN 454704-86-0 USPATFULL

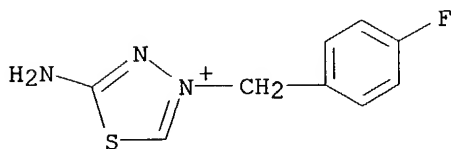
CN 1,3,4-Thiadiazolium, 5-amino-3-[(4-chlorophenyl)methyl]-, chloride (9CI)
(CA INDEX NAME)



● Cl⁻

RN 454704-87-1 USPATFULL

CN 1,3,4-Thiadiazolium, 5-amino-3-[(4-fluorophenyl)methyl]-, bromide (9CI)
(CA INDEX NAME)



● Br⁻

L5 ANSWER 2 OF 5 USPATFULL on STN

AB Provided, among things, is a method of treating or ameliorating an indication of the invention in an animal, including a human, comprising administering an effective amount of a compound of formula I: ##STR1##

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

ACCESSION NUMBER: 2003:4153 USPATFULL

TITLE: Method for treating fibrotic diseases or other indications VI

DELACROIX

INVENTOR(S): Gall, Martin, Morristown, NJ, UNITED STATES
 PATENT ASSIGNEE(S): Alteon, Inc., Ramsey, NJ, UNITED STATES (U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 2003004194	A1	20030102
	US 6596745	B2	20030722
APPLICATION INFO.:	US 2002-158344	A1	20020530 (10)

	NUMBER	DATE
PRIORITY INFORMATION:	US 2001-294438P	20010530 (60)
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	APPLICATION	
LEGAL REPRESENTATIVE:	ALLEN BLOOM, C/O DECHERT, PRINCETON PIKE CORPORATION CENTER, P.O. BOX 5218, PRINCETON, NJ, 08543-5218	
NUMBER OF CLAIMS:	23	
EXEMPLARY CLAIM:	1	
LINE COUNT:	1243	

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

DETD [0068] The effect of diabetes on the **eye** is called diabetic retinopathy and involves changes to the circulatory system of the retina. The earliest phase of the disease. . . ameliorate diabetic retinopathy. The first agents can be administered by the methods described below, including by topical administration to the **eye**. The agents can also be administered by intravitreal implant.

DETD [0114] Compositions can also be used to deliver the compound to the site where activity is desired; such as **eye** drops, gels and creams for **ocular** disorders.

DETD . . . compositions of this invention include aqueous solutions comprising a safe and effective amount of a subject compound intended for topical **intraocular** administration. Such compositions preferably comprise from about 0.01% to about 0.8% w/v of a subject compound, more preferably from about . . .

DETD [0119] The compounds of the invention are administered by **ocular**, oral, parenteral, including, for example, using formulations suitable as **eye** drops. For **ocular** administration, ointments or droppable liquids may be delivered by **ocular** delivery systems known to the art such as applicators or **eye** droppers. Such compositions can include mucomimetics such as hyaluronic acid, chondroitin sulfate, hydroxypropyl methylcellulose or polyvinyl alcohol, preservatives such as. . .

IT 477252-66-7P 477252-67-8P 477252-68-9P 477252-69-0P
477252-70-3P 477252-71-4P 477252-72-5P
477252-73-6P 477252-74-7P 477252-75-8P 477252-76-9P
 477252-77-0P 477252-78-1P 477252-79-2P 477252-80-5P
477252-81-6P 477252-82-7P 477252-83-8P
477252-84-9P 477252-85-0P 477252-86-1P 477252-87-2DP,
 derivs.

(method for treating fibrotic diseases or other indications)

IT **477252-70-3P 477252-71-4P 477252-72-5P**
477252-73-6P 477252-81-6P 477252-82-7P
477252-83-8P 477252-84-9P

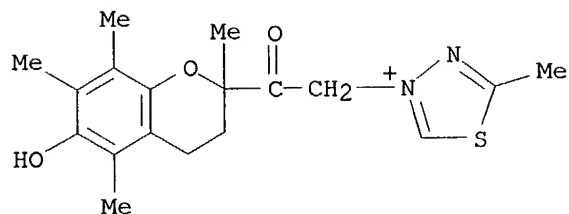
(method for treating fibrotic diseases or other indications)

RN 477252-70-3 USPATFULL

CN 1,3,4-Thiadiazolium, 3-[2-(3,4-dihydro-6-hydroxy-2,5,7,8-tetramethyl-2H-1-

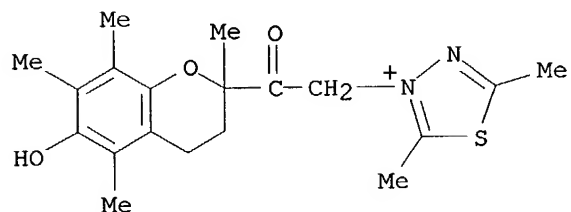
10/038,114

benzopyran-2-yl)-2-oxoethyl]-5-methyl- (9CI) (CA INDEX NAME)



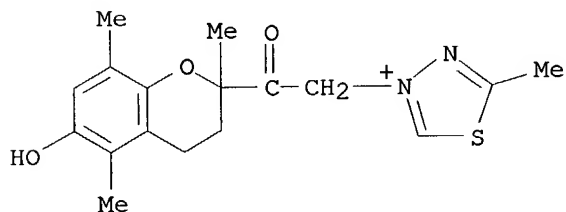
RN 477252-71-4 USPATFULL

CN 1,3,4-Thiadiazolium, 3-[2-(3,4-dihydro-6-hydroxy-2,5,7,8-tetramethyl-2H-1-benzopyran-2-yl)-2-oxoethyl]-2,5-dimethyl- (9CI) (CA INDEX NAME)



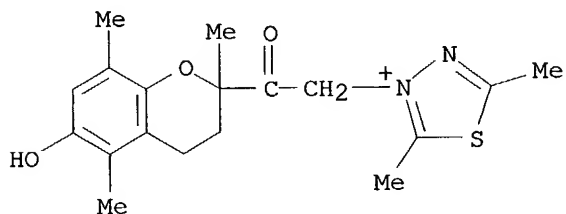
RN 477252-72-5 USPATFULL

CN 1,3,4-Thiadiazolium, 3-[2-(3,4-dihydro-6-hydroxy-2,5,8-trimethyl-2H-1-benzopyran-2-yl)-2-oxoethyl]-5-methyl- (9CI) (CA INDEX NAME)



RN 477252-73-6 USPATFULL

CN 1,3,4-Thiadiazolium, 3-[2-(3,4-dihydro-6-hydroxy-2,5,8-trimethyl-2H-1-benzopyran-2-yl)-2-oxoethyl]-2,5-dimethyl- (9CI) (CA INDEX NAME)

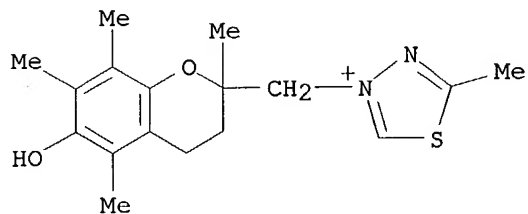


DELACROIX

10/038,114

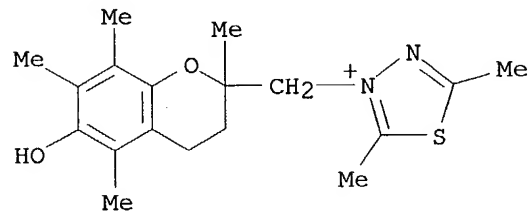
RN 477252-81-6 USPATFULL

CN 1,3,4-Thiadiazolium, 3-[(3,4-dihydro-6-hydroxy-2,5,7,8-tetramethyl-2H-1-benzopyran-2-yl)methyl]-5-methyl- (9CI) (CA INDEX NAME)



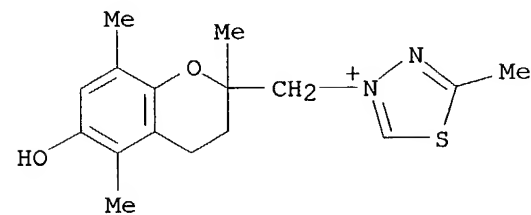
RN 477252-82-7 USPATFULL

CN 1,3,4-Thiadiazolium, 3-[(3,4-dihydro-6-hydroxy-2,5,7,8-tetramethyl-2H-1-benzopyran-2-yl)methyl]-2,5-dimethyl- (9CI) (CA INDEX NAME)



RN 477252-83-8 USPATFULL

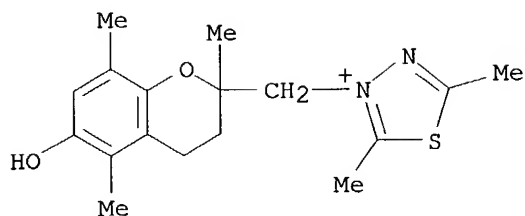
CN 1,3,4-Thiadiazolium, 3-[(3,4-dihydro-6-hydroxy-2,5,8-trimethyl-2H-1-benzopyran-2-yl)methyl]-5-methyl- (9CI) (CA INDEX NAME)



RN 477252-84-9 USPATFULL

CN 1,3,4-Thiadiazolium, 3-[(3,4-dihydro-6-hydroxy-2,5,8-trimethyl-2H-1-benzopyran-2-yl)methyl]-2,5-dimethyl- (9CI) (CA INDEX NAME)

DELACROIX



L5 ANSWER 3 OF 5 USPTAFULL on STN

AB Provided is a method of treating or ameliorating certain fibrotic diseases or other indications in an animal, including a human, comprising administering an effective amount of a compound of the formula I:

Y--Ar.sym..multidot.X.sup.--

wherein:

a. Ar is a five or six membered heteroaryl ring having a first ring nitrogen and optionally second or third ring nitrogens, with the remaining ring atoms being carbon, oxygen, or sulfur, provided the first nitrogen of Ar is a quaternary nitrogen and Ar is not thiazolium, oxazolium or imidazolium;

b. Y is substituted on the first ring nitrogen, with the proviso that if Ar is pyrazole, indazole, (1,2,3)-triazole, benzotriazole, or (1,2,4)-triazole, the second ring nitrogen is substituted

C. Y is:

1. a group of the formula --CH(R^{sup.5})--R^{sup.6} [as preferred in one embodiment]

(a) wherein R^{sup.5} is hydrogen, alkyl, cycloalkyl-, alkenyl-, alkynyl-, aminoalkyl-, hydroxy[C_{sub.1} to C_{sub.6}]-alkyl, dialkylaminoalkyl-, (N-[C_{sub.6} or C_{sub.10}]-aryl)(N-alkyl)aminoalkyl-, piperidin-1-ylalkyl-, pyrrolidin-1-ylalkyl, azetidinyllalkyl, 4-alkylpiperazin-1-ylalkyl, 4-alkylpiperidin-1-ylalkyl, 4-[C_{sub.6} or C_{sub.10}]-aryl piperazin-1-ylalkyl, 4-[C_{sub.6} or C_{sub.10}]-aryl piperidin-1-ylalkyl, azetidin-1-ylalkyl, morpholin-4-ylalkyl, thiomorpholin-4-ylalkyl, piperazin-1-ylalkyl, piperidin-1-ylalkyl, [C_{sub.6} or C_{sub.10}]-aryl, or independently the same as R^{sup.6};

(b) wherein R^{sup.6} is

(1) hydrogen, alkyl (which may be substituted by alkoxy carbonyl)-, alkenyl, alkynyl, cyano-, cyanoalkyl-, or Rs, wherein Rs is a [C_{sub.6} or C_{sub.10}]-aryl or a heterocycle containing 4-10 ring atoms of which 1-3 are heteroatoms selected from the group consisting of oxygen, nitrogen and sulfur; or

(2) a group of the formula --W--R^{sup.7} [as preferred in one embodiment], wherein R^{sup.7} is alkyl, alkoxy, hydroxy, or Rs [as preferred in one embodiment], wherein W is --C(.dbd.O)-- or

--S(O).sub.2--;

(3) a group of the formula --W--OR.sup.8 wherein R.sup.8 is hydrogen or alkyl,

(4) a group of the formula --CH(OH)Rs; or

(5) a group of the formula --W--N(R.sup.9)R.sup.10, wherein

(a) R.sup.9 is hydrogen and R.sup.10 is an alkyl or cycloalkyl, optionally substituted; or

(b) R.sup.9 is hydrogen or alkyl and R.sup.10 is Ar; or

(c) R.sup.9 is hydrogen or alkyl, R.sup.10 is a heterocycle containing 4-10 ring atoms of which 1-3 are heteroatoms are selected from the group consisting of oxygen, nitrogen and sulfur; or

(d) R.sup.9 and R.sup.10 are both alkyl groups; or

(e) R.sup.9 and R.sup.10 together with N form a heterocycle containing 4-10 ring atoms which can incorporate up to one additional heteroatom selected from the group of N, O or S in the ring, wherein the heterocycle is optionally substituted; or

(f) R.sup.9 and R.sup.10 are both hydrogen; or

2. --NH.sub.2, and

e. X is a pharmaceutically acceptable anion, which may be absent if the compound provides a neutralizing salt, or

(B) a pharmaceutically acceptable salt of the compound.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

ACCESSION NUMBER: 2002:323196 USPTAFULL

TITLE: Method for treating fibrotic diseases or other indications IIIC

INVENTOR(S): Wagle, Dilip, New York, NY, UNITED STATES
Gall, Martin, Morristown, NJ, UNITED STATES
Bell, Stanley C., Narberth, PA, UNITED STATES
LaVoie, Edmond J., Princeton Junction, NJ, UNITED STATES

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 2002183365	A1	20021205
APPLICATION INFO.:	US 2001-36857	A1	20011231 (10)

	NUMBER	DATE
PRIORITY INFORMATION:	US 2001-296246P	20010606 (60)
	US 2001-259238P	20010102 (60)
	US 2000-259294P	20001229 (60)

DOCUMENT TYPE: Utility

FILE SEGMENT: APPLICATION

LEGAL REPRESENTATIVE: ALLEN BLOOM, C/O DECHERT, PRINCETON PIKE CORPORATION

CENTER, P.O. BOX 5218, PRINCETON, NJ, 08543-5218

NUMBER OF CLAIMS: 49

EXEMPLARY CLAIM: 1

LINE COUNT: 3334

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

SUMM [0105] The effect of diabetes on the **eye** is called diabetic retinopathy and involves changes to the circulatory system of the retina. The earliest phase of the disease. . . phases of the disease, continued abnormal vessel growth and scar tissue may cause serious problems such as retinal detachment and **glaucoma**. First agents are used to treat, prevent, reduce or ameliorate diabetic retinopathy. The agents can be administered by the methods described below, including by topical administration to the **eye**. The agents can also be administered by intravitreal implant.

SUMM [0122] Pharmaceutical compositions of the invention include administering an **intraocular** pressure decreasing amount of a compound of the formula I.

SUMM [0320] Compositions can also be used to deliver the compound to the site where activity is desired; such as **eye** drops, gels and creams for **ocular** disorders.

SUMM . . . compositions of this invention include aqueous solutions comprising a safe and effective amount of a subject compound intended for topical **intraocular** administration. Such compositions preferably comprise from about 0.01% to about 0.8% w/v of a subject compound, more preferably from about. . .

SUMM [0325] The compounds of the invention are administered by **ocular**, oral, parenteral, including, for example, using formulations suitable as **eye** drops. For **ocular** administration, ointments or droppable liquids may be delivered by **ocular** delivery systems known to the art such as applicators or **eye** droppers. Such compositions can include mucomimetics such as hyaluronic acid, chondroitin sulfate, hydroxypropyl methylcellulose or polyvinyl alcohol, preservatives such as. . .

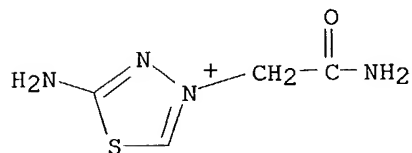
IT 13076-43-2P 63828-55-7P **454704-85-9P 454704-86-0P**
454704-87-1P 454704-88-2P 454704-89-3P 454704-90-6P
 454704-91-7P

(preparation of thiadiazolium, pyridinium and pyrimidinium salts for treating fibrotic diseases)

IT **454704-85-9P 454704-86-0P 454704-87-1P**
 (preparation of thiadiazolium, pyridinium and pyrimidinium salts for treating fibrotic diseases)

RN 454704-85-9 USPATFULL

CN 1,3,4-Thiadiazolium, 5-amino-3-(2-amino-2-oxoethyl)-, bromide (9CI) (CA INDEX NAME)

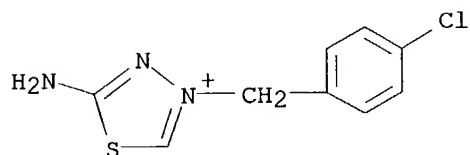


● Br⁻

10/038,114

RN 454704-86-0 USPATFULL

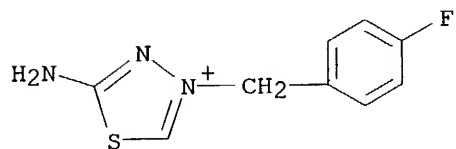
CN 1,3,4-Thiadiazolium, 5-amino-3-[(4-chlorophenyl)methyl]-, chloride (9CI)
(CA INDEX NAME)



● Cl⁻

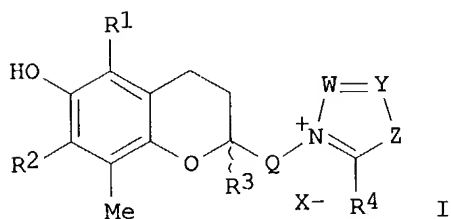
RN 454704-87-1 USPATFULL

CN 1,3,4-Thiadiazolium, 5-amino-3-[(4-fluorophenyl)methyl]-, bromide (9CI)
(CA INDEX NAME)



● Br⁻

L5 ANSWER 4 OF 5 HCAPLUS COPYRIGHT 2004 ACS on STN
GI



AB Provided, among things, is a method of treating or ameliorating an indication of the invention in an animal, including a human, comprising administering an effective amount of a compound of formula I, wherein: W and Y are independently N or, resp., CRW or CRY; Z is O, S or NRZ; Q is -CH2- or -(CO)-CH2-, where the methylene is bounded to a ring nitrogen; RW and RY are independently hydrogen, alkyl, -C.tplbond.CRE, -CH2-C.tplbond.CRP, aryl, alkylamino, arylamino, C(O)NH3, S(O)2NH2, etc.; RZ is alkyl,

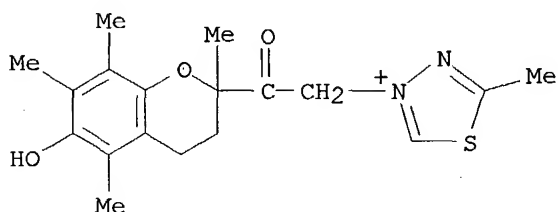
DELACROIX

(Uses)

(method for treating fibrotic diseases or other indications)

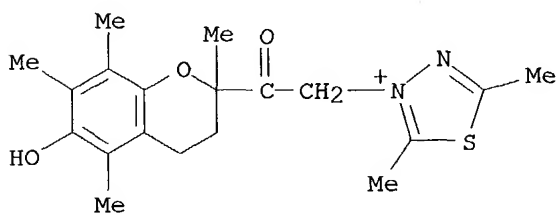
RN 477252-70-3 HCAPLUS

CN 1,3,4-Thiadiazolium, 3-[2-(3,4-dihydro-6-hydroxy-2,5,7,8-tetramethyl-2H-1-benzopyran-2-yl)-2-oxoethyl]-5-methyl- (9CI) (CA INDEX NAME)



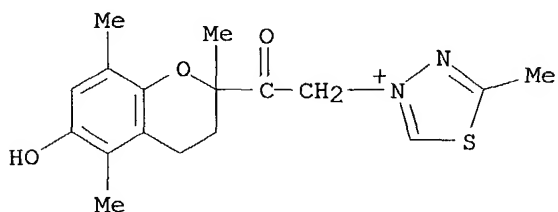
RN 477252-71-4 HCAPLUS

CN 1,3,4-Thiadiazolium, 3-[2-(3,4-dihydro-6-hydroxy-2,5,7,8-tetramethyl-2H-1-benzopyran-2-yl)-2-oxoethyl]-2,5-dimethyl- (9CI) (CA INDEX NAME)



RN 477252-72-5 HCAPLUS

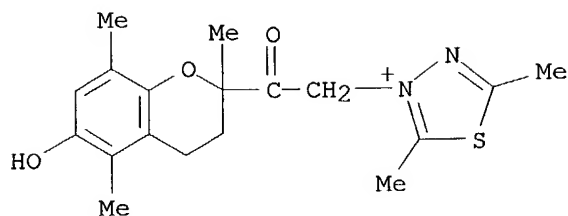
CN 1,3,4-Thiadiazolium, 3-[2-(3,4-dihydro-6-hydroxy-2,5,8-trimethyl-2H-1-benzopyran-2-yl)-2-oxoethyl]-5-methyl- (9CI) (CA INDEX NAME)



RN 477252-73-6 HCAPLUS

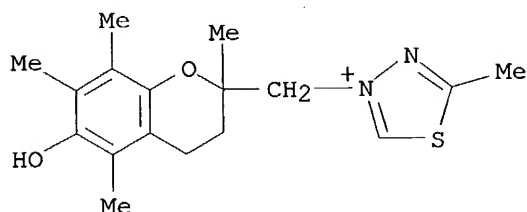
CN 1,3,4-Thiadiazolium, 3-[2-(3,4-dihydro-6-hydroxy-2,5,8-trimethyl-2H-1-benzopyran-2-yl)-2-oxoethyl]-2,5-dimethyl- (9CI) (CA INDEX NAME)

10/038,114



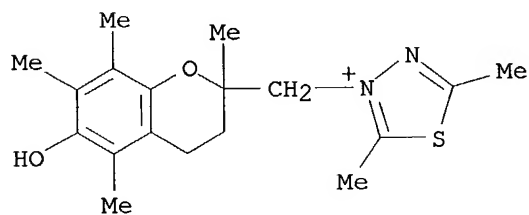
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CN 1,3,4-Thiadiazolium, 3-[(3,4-dihydro-6-hydroxy-2,5,7,8-tetramethyl-2H-1-benzopyran-2-yl)methyl]-5-methyl- (9CI) (CA INDEX NAME)



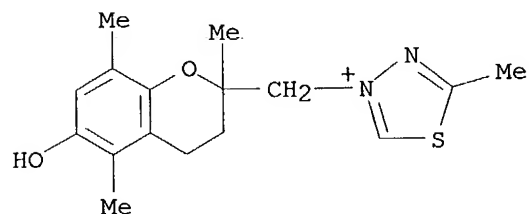
RN 477252-82-7 HCAPLUS

CN 1,3,4-Thiadiazolium, 3-[(3,4-dihydro-6-hydroxy-2,5,7,8-tetramethyl-2H-1-benzopyran-2-yl)methyl]-2,5-dimethyl- (9CI) (CA INDEX NAME)



RN 477252-83-8 HCAPLUS

CN 1,3,4-Thiadiazolium, 3-[(3,4-dihydro-6-hydroxy-2,5,8-trimethyl-2H-1-benzopyran-2-yl)methyl]-5-methyl- (9CI) (CA INDEX NAME)

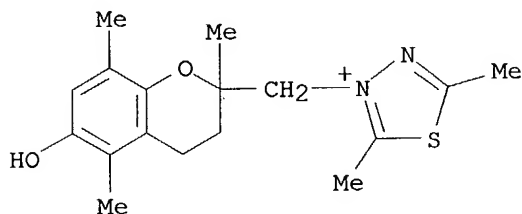


RN 477252-84-9 HCAPLUS

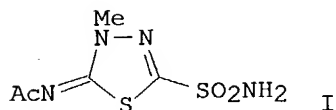
CN 1,3,4-Thiadiazolium, 3-[(3,4-dihydro-6-hydroxy-2,5,8-trimethyl-2H-1-

DELACROIX

benzopyran-2-yl)methyl]-2,5-dimethyl- (9CI) (CA INDEX NAME)



L5 ANSWER 5 OF 5 HCAPLUS COPYRIGHT 2004 ACS on STN
GI



AB The relation between physicochem. properties and lowering of **intraocular** pressure (IOP) was studied in rabbits after topical application of a series of 5-acylimino- and related imino-substituted analogs of methazolamide (Compound 4) (I). All the compds. had a KI vs. carbonic anhydrase C of about 10-8M. The parent methazolamide (5-acetyl) did not lower IOP, in contrast to the 5-CF₃ acetyl compound (Compound 28). The 5-propionyl compound (6) unexpectedly was 3 times more water soluble than methazolamide and had 10 times greater CHCl₃-buffer partition. The in vivo transcorneal permeability constant was 6 times greater than methazolamide. One h after 1 drop of a 2% suspension of Compound 6, anterior aqueous concentration (in micromolar) was 69 (for methazolamide, 8),

the

posterior aqueous concentration was 19 and concentration in the ciliary processes was 17.

The IOP dropped 2.2 mm Hg and returned to normal in 4 h. Other compds. in the series showed varying degrees of activity, ranging from Compound 28, which elicited an IOP fall of 3.5 mm Hg, to Compound 7, (n-pentyryl), for which the fall was 1.3 mm Hg. Also studied are substitutions for CH₃ on the ring N at position 4. There are multiple criteria for in vivo activity; a major factor is the balance between water and lipid solubility. The methazolamide analogs are compared with benzothiazole-2-sulfonamides, another class under investigation as topical carbonic anhydrase inhibitors designed to treat **glaucoma**.

ACCESSION NUMBER: 1987:546815 HCAPLUS

DOCUMENT NUMBER: 107:146815

TITLE: **Ocular** pharmacology of methazolamide analogs: distribution in the **eye** and effects on pressure after topical application

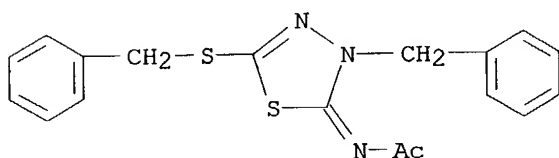
AUTHOR(S): Maren, Thomas H.; Bar-Ilan, Amir; Caster, Kenneth C.; Katritzky, Alan R.

CORPORATE SOURCE: Coll. Med., Univ. Florida, Gainesville, FL, 32610, USA
SOURCE: Journal of Pharmacology and Experimental Therapeutics

(1987), 241(1), 56-63
 CODEN: JPETAB; ISSN: 0022-3565

DOCUMENT TYPE: Journal
 LANGUAGE: English

- TI **Ocular** pharmacology of methazolamide analogs: distribution in the **eye** and effects on pressure after topical application
- AB The relation between physicochem. properties and lowering of **intraocular** pressure (IOP) was studied in rabbits after topical application of a series of 5-acylimino- and related imino-substituted analogs of methazolamide. . . solubility The methazolamide analogs are compared with benzothiazole-2-sulfonamides, another class under investigation as topical carbonic anhydrase inhibitors designed to treat **glaucoma**.
- ST methazolamide analog distribution **eye intraocular** pressure
- IT **Eye**
 (intraocular pressure of, methazolamide analogs effect on, distribution in)
- IT Biological transport
 (of methazolamide analogs, by **eye**, lipophilicity in relation to)
- IT Lipophilicity
 (of methazolamide analogs, distribution in **eye** in relation to)
- IT Molecular structure-biological activity relationship
 (intraocular pressure-reducing, of methazolamide analogs)
- IT 554-57-4, Methazolamide
 RL: BIOL (Biological study)
 (physicochem. properties and **ocular** pharmacol. of)
- IT 64387-67-3P 105339-30-8P 109014-82-6P 109480-58-2P
109480-59-3P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and conversion to sulfonamide of)
- IT 554-57-4DP, analogs 949-40-6P 952-59-0P 952-83-0P **965-11-7P**
 1081-57-8P 55217-95-3P 81428-88-8P 81428-89-9P 93745-70-1P
 93745-71-2P 109480-56-0P 109480-57-1P 109517-21-7P 109517-22-8P
 110501-80-9P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and physicochem. properties and **ocular** pharmacol. of)
- IT **109480-59-3P**
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and conversion to sulfonamide of)
- RN 109480-59-3 HCAPLUS
- CN Acetamide, N-[3-(phenylmethyl)-5-[(phenylmethyl)thio]-1,3,4-thiadiazol-2(3H)-ylidene]- (9CI) (CA INDEX NAME)



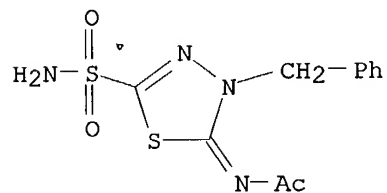
- IT **965-11-7P**
 RL: SPN (Synthetic preparation); PREP (Preparation)

10/038,114

(preparation and physicochem. properties and **ocular** pharmacol. of)

RN 965-11-7 HCAPLUS

CN Acetamide, N-[5-(aminosulfonyl)-3-(phenylmethyl)-1,3,4-thiadiazol-2(3H)-ylidene]- (9CI) (CA INDEX NAME)



=> fil reg

FILE 'REGISTRY' ENTERED AT 16:10:53 ON 23 JUN 2004

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STRUCTURE FILE UPDATES: 22 JUN 2004 HIGHEST RN 697737-72-7

DICTIONARY FILE UPDATES: 22 JUN 2004 HIGHEST RN 697737-72-7

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

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Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:

<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> d ide can tot l51

L51 ANSWER 1 OF 3 REGISTRY COPYRIGHT 2004 ACS on STN

RN 459165-10-7 REGISTRY

CN Pyridinium, 3-(aminocarbonyl)-1-[(4-methoxyphenyl)methyl]-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

MF C14 H15 N2 O2 . C F3 O3 S

SR CA

LC STN Files: CA, CAPLUS, CASREACT, USPAT2, USPATFULL

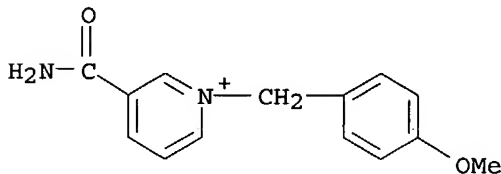
DT.CA CAPLUS document type: Patent

RL.P Roles from patents: PREP (Preparation); PRP (Properties)

CM 1

CRN 175979-55-2

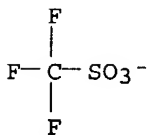
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CM 2

CRN 37181-39-8

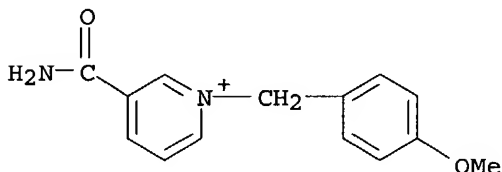
CMF C F3 O3 S



1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 137:228603

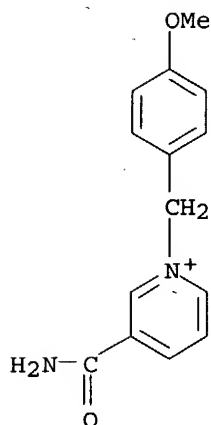
L51 ANSWER 2 OF 3 REGISTRY COPYRIGHT 2004 ACS on STN
RN 175979-55-2 REGISTRY
CN Pyridinium, 3-(aminocarbonyl)-1-[(4-methoxyphenyl)methyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C14 H15 N2 O2
CI COM
SR CA
LC STN Files: CA, CAPLUS
DT.CA Caplus document type: Journal
RL.NP Roles from non-patents: PROC (Process); PRP (Properties); RACT (Reactant or reagent)



1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 124:316412

L51 ANSWER 3 OF 3 REGISTRY COPYRIGHT 2004 ACS on STN
RN 63828-55-7 REGISTRY
CN Pyridinium, 3-(aminocarbonyl)-1-[(4-methoxyphenyl)methyl]-, chloride (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 3-Carbamoyl-1-(p-methoxybenzyl)pyridinium chloride (7CI)
OTHER NAMES:
CN N-4'-Methoxybenzylpyridinium chloride
MF C14 H15 N2 O2 . Cl
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, USPATFULL (*File contains numerically searchable property data)
DT.CA Caplus document type: Journal; Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)
RL.NP Roles from non-patents: PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent)
CRN (175979-55-2)



● Cl⁻

8 REFERENCES IN FILE CA (1907 TO DATE)
 8 REFERENCES IN FILE CAPLUS (1907 TO DATE)
 1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 137:216955
 REFERENCE 2: 125:300276
 REFERENCE 3: 113:22794
 REFERENCE 4: 108:166806
 REFERENCE 5: 103:22428
 REFERENCE 6: 99:104507
 REFERENCE 7: 98:61940
 REFERENCE 8: 87:80366

=> d his l51-

(FILE 'REGISTRY' ENTERED AT 16:01:53 ON 23 JUN 2004)
 L51 3 S L49,L50

FILE 'HCAOLD' ENTERED AT 16:09:07 ON 23 JUN 2004
 L52 1 S L51
 SEL AN
 EDIT /AN /OREF

FILE 'HCAPLUS' ENTERED AT 16:09:38 ON 23 JUN 2004
 L53 2 S E1
 L54 1 S L53 NOT GRUDZINSKA ?/AU
 L55 10 S L51

FILE 'USPATFULL, USPAT2' ENTERED AT 16:10:19 ON 23 JUN 2004
 L56 4 S L51

FILE 'REGISTRY' ENTERED AT 16:10:53 ON 23 JUN 2004

=> fil hcaold

FILE 'HCAOLD' ENTERED AT 16:11:07 ON 23 JUN 2004

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FILE COVERS 1907-1966

FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

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=> d l52 all hitstr

L52 ANSWER 1 OF 1 HCAOLD COPYRIGHT 2004 ACS on STN

AN CA59:9970a CAOLD

TI action of base on quaternary salts of nicotinamide

AU Dittmer, Donald C.; Kolyer, J. M.

IT 952-92-1 1652-58-0 1893-57-8 2996-08-9 4533-64-6 5096-13-9

6621-73-4 6951-52-6 13502-54-0 19355-18-1 **63828-55-7**

75340-29-3 92578-90-0 93807-08-0 93897-69-9 93946-35-1 94379-06-3

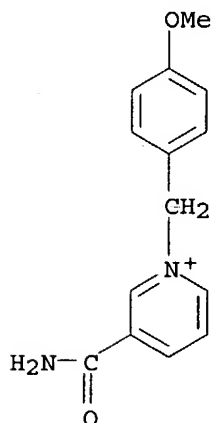
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IT **63828-55-7**

RN 63828-55-7 HCAOLD

CN Pyridinium, 3-(aminocarbonyl)-1-[(4-methoxyphenyl)methyl]-, chloride (9CI)
(CA INDEX NAME)



● Cl⁻

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FILE COVERS 1907 - 23 Jun 2004 VOL 140 ISS 26
FILE LAST UPDATED: 22 Jun 2004 (20040622/ED)
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This file contains CAS Registry Numbers for easy and accurate substance identification.

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L57          11 L54 OR L55
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=> d all hitstr tot
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L57 ANSWER 1 OF 11 HCAPLUS COPYRIGHT 2004 ACS on STN
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AN 2002:716518 HCAPLUS
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DN 137:228603
```

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ED Entered STN: 20 Sep 2002
```

```
TI NAD(P) mimic for use in enzymic redox reactions
```

```
IN Fish, Richard H.; Kerr, John B.; Lo, Christine H.
```

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PA The Regents of the University of California, USA
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SO PCT Int. Appl., 63 pp.
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CODEN: PIXXD2
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DT Patent
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LA English
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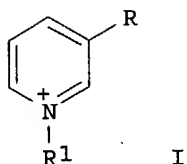
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CC 7-3 (Enzymes)
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FAN.CNT 1
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PI	WO 2002072869	A2	20020919	WO 2002-US7444	20020311
	WO 2002072869	A3	20030227		
	W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
	RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
	US 2003022266	A1	20030130	US 2001-805726	20010312
	US 6716596	B2	20040406		
	EP 1373552	A2	20040102	EP 2002-725121	20020311
	R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR			
PRAI	US 2001-805726	A	20010312		
	WO 2002-US7444	W	20020311		

OS CASREACT 137:228603; MARPAT 137:228603

GI



- AB Novel agents acting as co-factors for replacement of NAD(P)⁺/NAD(P)H co-enzyme systems in enzymic redox reactions are disclosed. A composition for replacement or regeneration of an NAD(P)⁺/NAD(P)H system in redox processes comprising (a) a polymer matrix, (b) a catalyst precursor, (3) a cofactor, and (d) an enzyme is further disclosed. The NAD(P) mimics are I [R = CN, CONH₂, CONHMe, CSNH₂, COCH₃, COOMe; R₁ = CH₂(CH₂O)_nYR₂, ribose-YR₂, or (X substituted)benzyl; Y = OP(:O)O, OBO₂, OSO₂, NHMe, (CH₂)_nNH, adenine, imidazole; R₂ = H, Me, (OCH₂CH₂)_n, (NCH₂CH₂)_n, [N:P(OMe)₂]_n; X = OMe, CF₃, (OCH₂CH₂)_n, OP(:O)OR₃; R₃ = H, Me, (OCH₂CH₂)_n, (NCH₂CH₂)_n, [N:P(OMe)₂]_n; n = 1-2000] and salts thereof. Thus, I with R₁ = benzyl and R = various substituents such as CONH₂ as well as I with R₁ = ribose 5'-methylphosphate and R = CONH₂ were synthesized and studied. Both of these coAlc. dehydrogenase enzyme mimics were used by horse liver alc. dehydrogenase to reduce phenethylmethylketone to the corresponding alc. with >93% ee (S-enantiomer). The reduced mimics were produced in this reaction using [Cp*Rh(bpy)(H₂O)](OTf)₂ as a catalyst precursor and sodium formate as hydride source.
- ST pyridinium deriv NAD NADP mimic enzymic oxidn redn
- IT 1445-91-6P 22148-86-3P 26184-62-3P 61277-90-5P 74709-08-3P
459165-24-3P
RL: BPN (Biosynthetic preparation); BIOL (Biological study); PREP (Preparation)
(NAD(P) mimic for use in enzymic redox reactions)
- IT 9031-72-5, Alcohol dehydrogenase 9035-73-8, Oxidase 9037-80-3, Reductase
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(NAD(P) mimic for use in enzymic redox reactions)
- IT 100-44-7P, Benzyl chloride, biological studies 237417-60-6P
237417-65-1P 416846-01-0P 416846-02-1P 459165-14-1P
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(NAD(P) mimic for use in enzymic redox reactions)
- IT 388078-51-1P 459165-10-7P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(NAD(P) mimic for use in enzymic redox reactions)
- IT 93-60-7 98-86-2, Phenylmethylketone, reactions 98-92-0, Nicotinamide
100-54-9, 3-Cyanopyridine 107-87-9, Methyl ethylketone 108-99-6,
3-Methylpyridine 350-03-8, 3-Acetyl pyridine 366-18-7, 2,2'-Bipyridyl
1007-32-5, Benzylethylketone 1094-61-7 2550-26-7,
Phenethylmethylketone 2630-41-3 4621-66-3, Thionicotinamide
29583-35-5 53830-52-7, 3-Pyridinecarbothioamide, n-methyl- 70887-29-5,
p-Methoxybenzyl iodide 165751-23-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(NAD(P) mimic for use in enzymic redox reactions)
- IT 6456-44-6P 194208-27-0P 237417-62-8P 237417-63-9P 237417-66-2P
237417-67-3P 237417-68-4P 237417-69-5P 237426-33-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(NAD(P) mimic for use in enzymic redox reactions)
- IT 53-59-8, NADP 53-84-9, NAD

RL: BSU (Biological study, unclassified); BIOL (Biological study)
(mimics; NAD(P) mimic for use in enzymic redox reactions)

IT 459165-10-7P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(NAD(P) mimic for use in enzymic redox reactions)

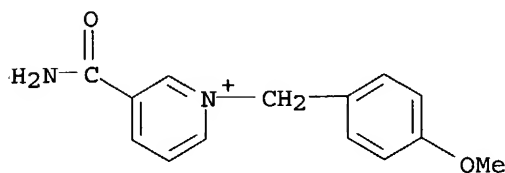
RN 459165-10-7 HCAPLUS

CN Pyridinium, 3-(aminocarbonyl)-1-[(4-methoxyphenyl)methyl]-, salt with
trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 175979-55-2

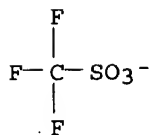
CMF C14 H15 N2 O2



CM 2

CRN 37181-39-8

CMF C F3 O3 S



L57 ANSWER 2 OF 11 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 2002:675770 HCAPLUS

DN 137:216955

ED Entered STN: 08 Sep 2002

TI Method for treating fibrotic diseases or other indications using
thiadiazolium, pyridinium and pyrimidinium salts

IN Wagle, Dilip; Gall, Martin; Bell, Stanley C.; Lavoie, Edmond J.

PA Alteon, Inc., USA

SO PCT Int. Appl., 104 pp.

CODEN: PIXXD2

DT Patent

LA English

IC ICM A61K

CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 1

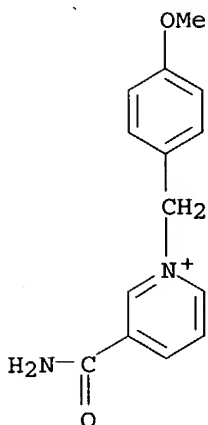
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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	WO 2002067851	A3	20030206		

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CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT,
RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ,

VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH,
 CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,
 BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
 EP 1355645 A2 20031029 EP 2001-273859 20011228
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
 IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
 US 2002183365 A1 20021205 US 2001-36857 20011231
 US 2004097495 A1 20040520 US 2003-691839 20031023
 PRAI US 2000-259294P P 20001229
 US 2001-259238P P 20010102
 US 2001-296246P P 20010606
 WO 2001-US49833 W 20011228
 US 2001-36857 A1 20011231
 OS MARPAT 137:216955
 AB The title compds. YAr+X- [I; Ar = 5-6 membered heteroaryl ring having a
 first ring N atom and optionally second or third ring N atoms, with the
 remaining ring atoms being C, O, or S, (provided the first N atom of Ar is
 a quaternary N and Ar is not thiazolium, oxazolium or imidazolium); Y is
 substituted on the first ring N atom (with the proviso that if Ar is
 pyrazole, indazole, triazole, benzotriazole, the second ring N atom is
 substituted with alkyl, alkoxy carbonylalkylene, aryl, etc.); Ar can be
 substituted on ring C atoms with aryl, carbamoyl, aralkyl, etc.; Y =
 CHR5R6 (R5 = H, alkyl, cycloalkyl, etc.; R6 = H, alkyl, alkenyl, etc.); X
 = a pharmaceutically acceptable anion, which may be absent if the compound
 provides a neutralizing salt], useful in treating or ameliorating certain
 fibrotic diseases or other indications linked to or associated with the
 formation of excess collagen, in an animal, including a human, were prepared
 Thus, refluxing 2-aminothiadiazole with 2-bromoacetamide in MeCN for 5 h
 afforded 5-amino-3-carbamoylmethyl-[1,3,4]thiadiazolium bromide. Assays
 to determine the activity of compds. I in breaking, reversing or inhibiting the
 formation of advanced glycosylation end products (AGEs) or AGE-mediated
 cross-links was presented (no data).
 ST thiadiazolium pyridinium pyrimidinium salt prepn advanced glycosylation
 endproduct AGE; fibrosis thiadiazolium pyridinium pyrimidinium salt prepn
 IT Glycoproteins
 RL: BSU (Biological study, unclassified); BIOL (Biological study)
 (AGE (advanced glycosylation end product); preparation of thiadiazolium,
 pyridinium and pyrimidinium salts for reversing advanced glycosylation
 cross-links)
 IT Intestine, disease
 (Crohn's, treatment of; preparation of thiadiazolium, pyridinium and
 pyrimidinium salts for treating fibrotic diseases)
 IT Artery, disease
 (arteritis, treatment of temporal; preparation of thiadiazolium, pyridinium
 and pyrimidinium salts for treating fibrotic diseases)
 IT Prostate gland, disease
 (benign hyperplasia, treatment of; preparation of thiadiazolium, pyridinium
 and pyrimidinium salts for treating fibrotic diseases)
 IT Mammary gland, disease
 (fibrocystic, treatment of; preparation of thiadiazolium, pyridinium and
 pyrimidinium salts for treating fibrotic diseases)
 IT Liver, disease
 Lung, disease
 Skin, disease
 (fibrosis, treatment of; preparation of thiadiazolium, pyridinium and
 pyrimidinium salts for treating fibrotic diseases)
 IT Muscle, disease
 (hypertrophy, treatment of; preparation of thiadiazolium, pyridinium and
 pyrimidinium salts for treating fibrotic diseases)
 IT Intestine, disease
 (inflammatory, treatment of; preparation of thiadiazolium, pyridinium and
 pyrimidinium salts for treating fibrotic diseases)

- IT Connective tissue, disease
(mixed connective tissue disease, treatment of; preparation of thiadiazolium, pyridinium and pyrimidinium salts for treating fibrotic diseases)
- IT Muscle, disease
(myositis, treatment of; preparation of thiadiazolium, pyridinium and pyrimidinium salts for treating fibrotic diseases)
- IT Artery, disease
(periarteritis nodosa, treatment of; preparation of thiadiazolium, pyridinium and pyrimidinium salts for treating fibrotic diseases)
- IT Pleura, disease
(pleurisy, treatment of; preparation of thiadiazolium, pyridinium and pyrimidinium salts for treating fibrotic diseases)
- IT Anti-inflammatory agents
Human
(preparation of thiadiazolium, pyridinium and pyrimidinium salts for treating fibrotic diseases)
- IT Connective tissue, disease
(scleroderma, treatment of; preparation of thiadiazolium, pyridinium and pyrimidinium salts for treating fibrotic diseases)
- IT Nervous system, disease
(sclerosis, treatment of cerebroscclerosis, annular sclerosis, diffuse sclerosis and lobar sclerosis; preparation of thiadiazolium, pyridinium and pyrimidinium salts for treating fibrotic diseases)
- IT Cystic fibrosis
Fibrosis
Hypertrophy
Sarcoidosis
(treatment of; preparation of thiadiazolium, pyridinium and pyrimidinium salts for treating fibrotic diseases)
- IT Blood vessel, disease
(vasculitis, treatment of; preparation of thiadiazolium, pyridinium and pyrimidinium salts for treating fibrotic diseases)
- IT 13076-43-2P 63828-55-7P 454704-85-9P 454704-86-0P
454704-87-1P 454704-88-2P 454704-89-3P 454704-90-6P 454704-91-7P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of thiadiazolium, pyridinium and pyrimidinium salts for treating fibrotic diseases)
- IT 98-92-0, Nicotinamide 100-39-0, Benzyl bromide 104-83-6,
4-Chlorobenzyl chloride 289-95-2, Pyrimidine 456-04-2 459-46-1,
4-Fluorobenzyl bromide 589-17-3, 4-Bromobenzyl chloride 683-57-8,
2-Bromoacetamide 824-94-2, 4-Methoxybenzyl chloride 937-20-2,
2-Chloro-1-(4-chlorophenyl)ethanone 4005-51-0, 2-Aminothiadiazoole
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of thiadiazolium, pyridinium and pyrimidinium salts for treating fibrotic diseases)
- IT 63828-55-7P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of thiadiazolium, pyridinium and pyrimidinium salts for treating fibrotic diseases)
- RN 63828-55-7 HCAPLUS
CN Pyridinium, 3-(aminocarbonyl)-1-[(4-methoxyphenyl)methyl]-, chloride (9CI)
(CA INDEX NAME)



● Cl⁻

L57 ANSWER 3 OF 11 HCAPLUS COPYRIGHT 2004 ACS on STN
 AN 1996:619241 HCAPLUS
 DN 125:300276
 ED Entered STN: 18 Oct 1996
 TI Reactions of Charged Substrates. 5. The Solvolysis and Sodium Azide Substitution Reactions of Benzylpyridinium Ions in Deuterium Oxide
 AU Buckley, Neil; Oppenheimer, Norman J.
 CS Department of Pharmaceutical Chemistry, University of California, San Francisco, CA, 94143-0446, USA
 SO Journal of Organic Chemistry (1996), 61(21), 7360-7372
 CODEN: JOCEAH; ISSN: 0022-3263
 PB American Chemical Society
 DT Journal
 LA English
 CC 22-4 (Physical Organic Chemistry)
 Section cross-reference(s): 7
 AB Second-order rate consts. and activation values were measured for the reactions with NaN₃ of a series of 4-Y-substituted (Y = MeO, Me, H, Cl, and NO₂) benzyl 3'-Z-substituted (Z = CN, CONH₂, H, F, Ac) pyridinium chlorides in deuterium oxide. 3'-Cyanopyridine substrates reacted much faster than nicotinamide and pyridine substrates; in the pyridine series the 4-Me, 4-H, and 4-Cl benzyl analogs did not react for up to 6 mo at 96° in 1.7 M NaN₃. The 3'-cyanopyridine substrates do not exhibit borderline kinetic behavior, but the nicotinamide substrates do. The Hammett plot is flat for the NaN₃ reaction of 3'-cyanopyridine substrates and increasingly V-shaped for the nicotinamide and pyridine substrates. The values of ρ_{LG} (four-point plot) for the NaN₃ reaction of the 4-MeO benzyl substrates is -1.45, which is usually interpreted as being a very "late" activated complex. Two-point Bronsted "plots" for the other benzyl derivs. and for two N-methylpyridinium ions give values of ρ_{LG} in the same range. The second-order rate constant and activation values for N-methyl-3'-cyanopyridinium iodide are within the same range as those for the benzyl substrates. For the hydrolysis reaction, the Hammett plot is linear for 3'-cyanopyridine substrates ($\rho^+ = -1.24$) and flat for the nicotinamide substrates. The extent of hydrolysis of 0.005-0.05 M solns. of the 3'-cyanopyridine substrates depended on the initial concentration of substrate, and hydrolysis was slowed significantly or stopped completely in the presence of exogenous 3-cyanopyridine. These results show that an equilibrium is established among the products for the 4-MeO, 4-Me, 4-H, and

4-Cl substrates; the 4-NO₂ substrate reacted too slowly to discern any difference. Data for the extent of hydrolysis were fitted by an equation derived assuming the equilibrium. Despite this limitation on a classic test of mechanism, the rates and ρ values are consistent with direct displacement by solvent and not with a unimol. process. These results, which are rationalized in terms of the Pross-Shaik model, suggest that there are no ion-dipole complex intermediates in the benzyl series and show that borderline kinetic behavior is a function of leaving group ability and is not necessarily related to a change in mechanism. A computational approach was used to evaluate anomalous β LG values for the hydrolysis and nucleophilic substitution reactions of the methylpyridinium ion substrates. It was found that neither the Nu-substrate bond lengths nor the difference in charge matched the β LG values. The value of $\Delta\Delta S_{\text{thermod.}}$ of -15 gibbs/mol between (4-methoxybenzyl)-3'-cyanopyridinium chloride and the corresponding dimethylsulfonium chloride in the NaN₃ reaction, which is the result of the solvation of the pyridine at the transition state and the lack of solvation of SMe₂, is used to argue that the source of NAD⁺ glycohydrolase "catalysis" of NAD⁺ bond cleavage is the result of desolvation of the leaving group upon binding.

- ST benzylpyridinium hydrolysis azide substitution kinetics mechanism;
reaction const benzylpyridinium hydrolysis azide substitution; NAD
glycohydrolase catalysis
- IT Electron configuration and Electron density
Heat of hydrolysis
Hydrolysis
Kinetics of hydrolysis
Leaving group effects
Linear free energy relationship
Potential energy surface and hypersurface
Reaction constant
Substituent effect
Substitution reaction, nucleophilic
Transition state structure
(kinetics and mechanism of solvolysis and sodium azide substitution
reactions of benzylpyridinium ions)
- IT Pyridinium compounds
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT
(Reactant); PROC (Process); RACT (Reactant or reagent)
(kinetics and mechanism of solvolysis and sodium azide substitution
reactions of benzylpyridinium ions)
- IT Molecular orbital
(frontier, kinetics and mechanism of solvolysis and sodium azide
substitution reactions of benzylpyridinium ions)
- IT Heat of substitution reaction
Kinetics of substitution reaction
(nucleophilic, kinetics and mechanism of solvolysis and sodium azide
substitution reactions of benzylpyridinium ions)
- IT 2876-13-3
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT
(Reactant); PROC (Process); RACT (Reactant or reagent)
(estimated; kinetics and mechanism of solvolysis and sodium azide
substitution reactions of benzylpyridinium ions)
- IT 594-09-2, Trimethylphosphine 1004-16-6, 3-Cyano-1-methylpyridinium
iodide 4329-72-0 5096-13-9 6456-44-6 6621-73-4 6951-52-6
14343-69-2, Azide 14535-08-1 14535-12-7 20461-54-5, Iodide,
reactions 26628-22-8, Sodium azide 52354-19-5 63828-55-7
74796-72-8 76053-06-0 87976-56-5 98349-72-5 183054-49-1
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT
(Reactant); PROC (Process); RACT (Reactant or reagent)
(kinetics and mechanism of solvolysis and sodium azide substitution
reactions of benzylpyridinium ions)
- IT 7732-18-5, Water, reactions 15923-33-8 183054-50-4

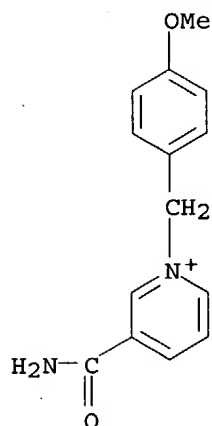
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent) (potential surface calcn.; kinetics and mechanism of solvolysis and sodium azide substitution reactions of benzyropyridinium ions)

IT 63828-55-7

RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent) (kinetics and mechanism of solvolysis and sodium azide substitution reactions of benzyropyridinium ions)

RN 63828-55-7 HCAPLUS

CN Pyridinium, 3-(aminocarbonyl)-1-[(4-methoxyphenyl)methyl]-, chloride (9CI) (CA INDEX NAME)



● Cl⁻

L57 ANSWER 4 OF 11 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1996:191937 HCAPLUS

DN 124:316412

ED Entered STN: 04 Apr 1996

TI Reactions of Charged Substrates. 4. The Gas-Phase Dissociation of (4-Substituted benzyl)dimethylsulfoniums and -pyridiniums

AU Buckley, Neil; Maltby, David; Burlingame, Alma L.; Oppenheimer, Norman J.

CS School of Pharmacy, University of California, San Francisco, CA, 94143-0446, USA

SO Journal of Organic Chemistry (1996), 61(8), 2753-62

CODEN: JOCEAH; ISSN: 0022-3263

PB American Chemical Society

DT Journal

LA English

CC 22-12 (Physical Organic Chemistry)

Section cross-reference(s): 33

AB The relative rates for the gas-phase dissociation $RX^+ \rightarrow R^+ + X^\circ$ of five (4-Y-substituted benzyl)dimethylsulfoniums (Y = MeO, Me, H, Cl, and NO₂) and 24 (4-Y-substituted benzyl)-3'-Z-pyridiniums (complete series for Z = CN, Cl, CONH₂, and H, and 4-methoxy- and 4-nitrobenzyls for Z = F and CH₃CO) were measured using liquid secondary ion mass spectrometry. The Hammett plot (vs δAG° or σ^+) is linear for the sulfoniums, but plots for the four pyridinium series have a drastic break between the 4-Cl and 4-NO₂ substrates. Broensted-like plots for the pyridiniums show a strong leaving group effect only for 4-nitrobenzyls. An anal. of these linear free energy relations with supporting evidence

from semiempirical computations suggests that collisionally activated pyridinium substrates dissociate through two pathways, direct dissociation and an ion-neutral complex intermediate. Comparison of these results with results for the solution reactions of some of these compds. shows that the mechanism is different in the gas and solution phases. Sufficient exptl. data are not available to assign a mechanism for dissociation to the sulfonium series, but computational results show characteristics of a direct dissociative mechanism.

ST disson gas phase benzyldimethylsulfonium benzyldimethylpyridinium; sulfonium benzyldimethyl gas phase disson; pyridinium benzyldimethyl gas phase disson

IT Linear free energy relationship
Reaction constant
(for gas-phase dissociation of substituted benzyldimethylsulfoniums and -pyridiniums)

IT Dissociation
Kinetics of dissociation
(kinetics and mechanism of gas-phase dissociation of substituted benzyldimethylsulfoniums and -pyridiniums)

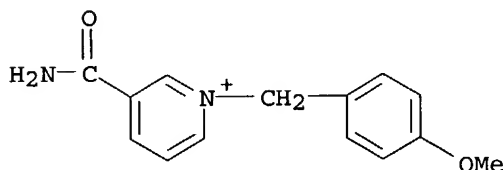
IT Leaving group effects
Substituent effect
(on gas-phase dissociation of substituted benzyldimethylsulfoniums and -pyridiniums)

IT Linear free energy relationship
(Broensted, for gas-phase dissociation of substituted benzyldimethylsulfoniums and -pyridiniums)

IT 15519-25-2 16183-83-8 16183-87-2 24837-70-5 38332-27-3
45809-04-9 45964-81-6 46122-80-9 46441-13-8 48120-95-2
58219-38-8 58219-39-9 71897-24-0 71897-27-3 78186-22-8
133227-04-0 175979-55-2 175979-56-3 175979-57-4
175979-58-5 175979-59-6 175979-60-9 175979-61-0 175979-62-1
175979-63-2 175979-64-3 175979-65-4 175979-66-5 175979-67-6
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(kinetics and mechanism of gas-phase dissociation of substituted benzyldimethylsulfoniums and -pyridiniums)

IT 175979-55-2
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(kinetics and mechanism of gas-phase dissociation of substituted benzyldimethylsulfoniums and -pyridiniums)

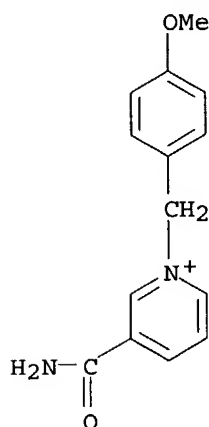
RN 175979-55-2 HCAPLUS
CN Pyridinium, 3-(aminocarbonyl)-1-[(4-methoxyphenyl)methyl]- (9CI) (CA INDEX NAME)



L57 ANSWER 5 OF 11 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1990:422794 HCAPLUS
DN 113:22794
ED Entered STN: 21 Jul 1990
TI Addition of cyanide ion to nicotinamide cations in acetonitrile. Formation of nonproductive charge-transfer complexes
AU Engbersen, Johan F. J.; Koudijs, Arie; Sleiderink, Hedwig M.; Franssen,

Maurice C. R.
CS Lab. Org. Chem., Agric. Univ., Wageningen, 6703 HB, Neth.
SO Journal of the Chemical Society, Perkin Transactions 2: Physical Organic
Chemistry (1972-1999) (1990), (1), 79-83
CODEN: JCPKBH; ISSN: 0300-9580
DT Journal
LA English
CC 22-4 (Physical Organic Chemistry)
OS CASREACT 113:22794
AB The mixing of equal vols. of 0.2 mmol dm⁻³ 1-benzylnicotinamide ion and 2
mmol dm⁻³ cyanide ion results in the immediate formation of a transient
absorption band at 375 nm which can be ascribed to a charge-transfer
complex. This complex disappears within ca. 0.2 s with the formation of
the 1,6-addition product which, in turn, is rapidly converted into the
thermodynamically more stable 1,4-adduct. Me substitution at the
6-position of the nicotinamide ring inhibits the formation of the
1,6-adduct, resulting in an increase in the lifetime of the
charge-transfer complex. Subsequently a mixture of the 1,4-cyanide adduct
and, most likely, the 1,2-adduct is formed. Rate effects with variation
of substituents in the 1-benzyl group reveal that charge-transfer complex
formation is counterproductive to the formation of addition products.
ST cyanide ion addn nicotinamide cation; charge transfer complex cyanide
nicotinamide; substituent effect cyanide addn nicotinamide
IT Reaction constant
(for addition, dissociation, and charge-transfer-complexation processes in
cyanide ion-nicotinamide cation systems)
IT Addition reaction
(of cyanide ion with nicotinamide cations, formation of nonproductive
charge-transfer complexes in)
IT Kinetics of addition reaction
(of cyanide ion with nicotinamide cations, solvent and substituent
effects on)
IT Kinetics of dissociation
(of cyanide-ion adducts with nicotinamide cations, solvent and
substituent effects on)
IT Ultraviolet and visible spectra
(of transient species, in addition reaction of cyanide ion with
nicotinamide cations)
IT Substituent effect
(on addition, dissociation, and charge-transfer-complexation processes in
cyanide ion-nicotinamide cation systems)
IT 151-50-8, Potassium cyanide (K(CN))
RL: RCT (Reactant); RACT (Reactant or reagent)
(addition reaction of, with nicotinamide cations)
IT 127678-22-2 127678-24-4 127678-25-5 127678-27-7 127678-29-9
RL: PROC (Process)
(decay of, kinetics of)
IT 13076-43-2P 54027-58-6P 63761-90-0P 63761-95-5P 63828-55-7P
70293-11-7P 127663-01-8P 127663-02-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation and addition reaction of, with cyanide)
IT 96551-72-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and charge-transfer complexation and addition reaction of, with
cyanide)
IT 127663-05-2P 127663-06-3P 127663-07-4P 127678-20-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and charge-transfer complexation of, with cyanide)
IT 19432-61-2P 75420-69-8P 75420-70-1P 75420-71-2P 75420-74-5P
127663-03-0P 127663-04-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and dissociation of, kinetics of)

IT 127663-08-5P 127663-09-6P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 IT 63828-55-7P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and addition reaction of, with cyanide)
 RN 63828-55-7 HCAPLUS
 CN Pyridinium, 3-(aminocarbonyl)-1-[(4-methoxyphenyl)methyl]-, chloride (9CI)
 (CA INDEX NAME)

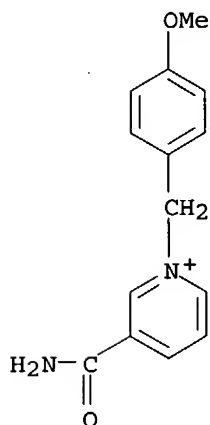


● Cl⁻

L57 ANSWER 6 OF 11 HCAPLUS COPYRIGHT 2004 ACS on STN
 AN 1988:166806 HCAPLUS
 DN 108:166806
 ED Entered STN: 13 May 1988
 TI Polarographic reduction of p-substituted 1-phenyl-3-(aminocarbonyl)pyridinium salts
 AU Krechl, Jiri; Mizaninoiva, Daniela; Volke, Jiri; Kuthan, Josef
 CS Dep. Org. Chem., Prague Inst. Chem. Technol., Prague, 166 28, Czech.
 SO Collection of Czechoslovak Chemical Communications (1987), 52(6), 1550-60
 CODEN: CCCCAK; ISSN: 0366-547X
 DT Journal
 LA English
 CC 22-7 (Physical Organic Chemistry)
 Section cross-reference(s): 72
 AB The substituent effect (H, NO₂, CO₂H, Br, Cl, NHAc, Me, OMe, OH, NEt₂) on the polarog. behavior of p-substituted 1-phenyl-3-aminocarbonylpyridinium cations has been investigated, in particular on their half-wave potentials in aqueous phosphate buffers pH 6.65 (10% DMF) and in anhydrous solns. of DMF with 0.05 mol L⁻¹ Bu₄N⁺ BF₄⁻ as supporting electrolyte. The half-wave potentials of the reduction wave which corresponds to the uptake of a single electron (wave B) and to the formation of the primary radical, obey a Hammett correlation in a way similar to the case of 1-benzyl-3-aminocarbonylpyridinium cations. The slope Q_{π,R} in the Hammett plot equals 0.093 V for 10% DMF and 0.179 V for anhydrous DMF and compares thus with the slope obtained with the 1-benzyl derivs. where 0.05 V was found for water and 0.127 V of anhydrous acetonitrile. The transfer of the substituent effect from the substituent in the para position on the benzene nucleus to the heterocyclic ring is

thus equally active in both substances and depends more strongly on the solvent than on the structure of the cation of both types. The low sensitivity in both series towards a change in the substituent is explained by the fact that during the uptake of the electron the benzene and the pyridine nucleus are not even approx. coplanar. This is why the π -overlap between the two nuclei is considerably restricted. The anal. of sampled d.c.-polarog. waves has confirmed that the one-electron uptake is followed by a chemical reaction, most probably a dimer formation or a reaction of the primary product with the starting substance.

ST polarog redn pyridinium salt; amidopyridinium phenyl electrochem redn LFER
 IT Reduction
 (of substituted phenyl(aminocarbonyl)pyridinium salts, substituent effects on)
 IT Substituent effect
 (on polarog. reduction of phenyl(aminocarbonyl)pyridinium salts)
 IT 5096-13-9 6951-52-6 52354-19-5 **63828-55-7**
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (polarog. reduction of)
 IT 54027-59-7P 54027-60-0P 69986-64-7P 76911-53-0P 76911-55-2P
 76911-56-3P 87384-49-4P 87384-51-8P 87384-52-9P 112445-86-0P
 113849-47-1P 113849-48-2P 113849-49-3P 113849-50-6P 113849-53-9P
 113849-54-0P 113849-55-1P 113849-57-3P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and polarog. reduction of)
 IT 98-92-0, Nicotinamide
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with anilines)
 IT 62-53-3, reactions 93-05-0 100-01-6, reactions 104-94-9,
 4-Methoxyaniline 106-40-1, 4-Bromoaniline 106-47-8, 4-Chloroaniline,
 reactions 106-49-0, reactions 122-80-5, 4-Acetamidoaniline 123-30-8,
 4-Hydroxyaniline 150-13-0, 4-Aminobenzoic acid
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with nicotinamide)
 IT **63828-55-7**
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (polarog. reduction of)
 RN 63828-55-7 HCAPLUS
 CN Pyridinium, 3-(aminocarbonyl)-1-[(4-methoxyphenyl)methyl]-, chloride (9CI)
 (CA INDEX NAME)

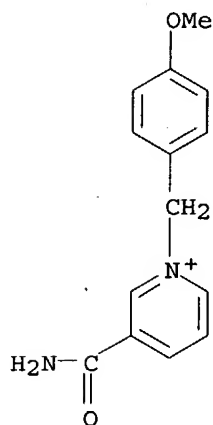


L57 ANSWER 7 OF 11 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1985:422428 HCAPLUS
DN 103:22428
ED Entered STN: 27 Jul 1985
TI Selective reduction of pyridinium, quinolinium, and pyrazinium salts to the dihydro stage with 1-benzyl-1,2-dihydroisonicotinamide
AU Nuvole, Antonio; Paglietti, Giuseppe; Sanna, Paolo; Acheson, R. Morrin
CS Ist. Chim. Farm., Univ. Sassari, Sassari, 07100, Italy
SO Journal of Chemical Research, Synopses (1984), (11), 356-7
CODEN: JRPSDC; ISSN: 0308-2342
DT Journal
LA English
CC 27-17 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 22, 28
OS CASREACT 103:22428
AB Quinolinium, pyridinium, and pyrazinium salts were reduced selectively to 1,4-dihydroquinolines, 1,4-dihydropyridines, and 1,6-dihydropyrazines, resp., by 1-benzyl-1,2-dihydroisonicotinamide (I) in dry MeOH under N. E.g., reduction of N-benzyl-3-carbamoylquinolinium bromide by I for 5 min gave N-benzyl-1,4-dihydroquinoline-3-carboxamide quant.
ST benzylisonicotinamide redn quinolinium pyridinium pyrazolinium; isonicotinamide benzyl redn quaternary compd; regioselective redn quaternary compd benzylisonicotinamide; quinolinium redn benzylisonicotinamide regioselective; pyridinium redn benzylisonicotinamide regioselective; pyrazinium redn benzylisonicotinamide regioselective
IT Regiochemistry
(of reduction of quinolinium, pyridinium, or pyrazinium compds. by benzyl-1,2-dihydroisonicotinamide)
IT Reduction
(regioselective, of quinolinium, pyridinium, and pyrazinium compds. by benzyl-1,2-dihydroisonicotinamide)
IT 62417-98-5P 96421-80-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and selective reduction of, by benzyl-1,2-dihydroisonicotinamide)
IT 96421-81-7P 96421-82-8P 96421-83-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT 952-92-1P 2288-38-2P 17260-79-6P 17750-23-1P 19350-64-2P
20224-92-4P 34865-02-6P 37589-77-8P 56133-30-3P 57355-62-1P
71127-33-8P 73027-91-5P 74124-15-5P 78224-91-6P 88928-67-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by selective reduction of quaternary compound with benzyl-1,2-dihydroisonicotinamide)
IT 100-39-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(quaternization by, of Me quinolinecarboxylate, cyanopyridine, and pyrazinecarboxamide)
IT 98-96-4 100-48-1 53951-84-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(quaternization of, by benzyl bromide)
IT 75532-98-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction by, of quinolinium, pyridinium, and pyrazinium compds., regioselective)
IT 5496-66-2 6456-44-6 6516-41-2 6516-53-6 13076-43-2 13958-90-2
26368-94-5 63828-55-7 70293-11-7 73027-90-4 96421-79-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction of, by benzyl-1,2-dihydroisonicotinamide, regioselective)
IT 63828-55-7

RL: RCT (Reactant); RACT (Reactant or reagent)
 (reduction of, by benzyldihydroisonicotinamide, regioselective)

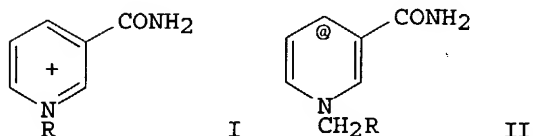
RN 63828-55-7 HCAPLUS

CN Pyridinium, 3-(aminocarbonyl)-1-[(4-methoxyphenyl)methyl]-, chloride (9CI)
 (CA INDEX NAME)



● Cl⁻

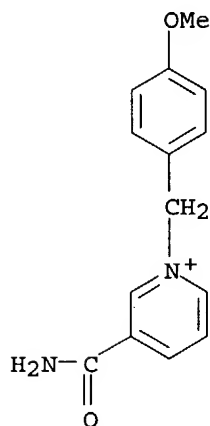
L57 ANSWER 8 OF 11 HCAPLUS COPYRIGHT 2004 ACS on STN
 AN 1983:504507 HCAPLUS
 DN 99:104507
 ED Entered STN: 12 May 1984
 TI Dihydropyridines. XLVIII. Substituent effect in addition of cyanide ion to p-substituted 1-benzyl-3-carbamoylpyridinium chlorides
 AU Pavlikova-Raclova, Frantiska; Kuthan, Josef
 CS Dep. Org. Chem., Prague Inst. Chem. Technol., Prague, 166 28/6, Czech.
 SO Collection of Czechoslovak Chemical Communications (1983), 48(5), 1401-7
 CODEN: CCCCAK; ISSN: 0366-547X
 DT Journal
 LA English
 CC 22-4 (Physical Organic Chemistry)
 GI



AB Rate consts. for the title reaction were determined in aqueous solns. of 8 quaternary salts of nicotinamide (I; R = p-XC₆H₄CH₂; X = MeO, Me, H, F, Cl, CO₂Me, cyano, NO₂). Good Hammett correlations were found, along with correlation of E_{1/2} of polarog. reduction of I with rate and equilibrium consts.

In aqueous media, reduction of I (same R; X = Me, H, F, Cl, MeO) with π -donor substituents proceeds via a simple E mechanism I \rightarrow II, whereas in the case of π -acceptor substituents (I; X = NO₂, CN, CO₂Me), radicals II are formed via a 3-step CEC mechanism.

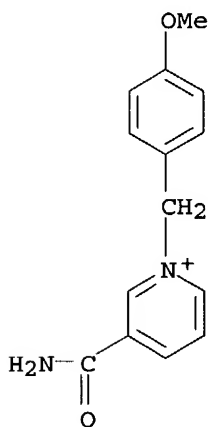
ST cyanation benzylcarbamoylpyridinium kinetics mechanism; LFER cyanation
benzylcarbamoylpyridinium
IT Linear free energy relationship
(in cyanation of benzylcarbamoylpyridinium chlorides)
IT Cyanation
(of benzylcarbamoylpyridinium chlorides, mechanism of)
IT Kinetics of cyanation
Reduction, electrochemical
(of benzylcarbamoylpyridinium chlorides)
IT 1652-58-0 5096-13-9 6621-73-4 6951-52-6 52354-19-5
63828-55-7 84354-35-8 84389-20-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyanation of, kinetics and mechanism of)
IT 63828-55-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyanation of, kinetics and mechanism of)
RN 63828-55-7 HCAPLUS
CN Pyridinium, 3-(aminocarbonyl)-1-[(4-methoxyphenyl)methyl]-, chloride (9CI)
(CA INDEX NAME)



● Cl⁻

L57 ANSWER 9 OF 11 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1983:61940 HCAPLUS
DN 98:61940
ED Entered STN: 12 May 1984
TI Polarographic reduction of p-substituted 1-benzyl-3-carbamoylpyridinium
chlorides
AU Kuthan, Josef; Pavlikova-Raclova, Frantiska
CS Dep. Org. Chem., Prague Inst. Chem. Technol., Prague, 166 28/6, Czech.
SO Collection of Czechoslovak Chemical Communications (1982), 47(11),
2890-903
CODEN: CCCCAK; ISSN: 0366-547X
DT Journal
LA English
CC 72-2 (Electrochemistry)
AB Substituent effects (H, NO₂, CN, CO₂Me, Me, MeO, Me₂N, Cl, F) on polarog.
characteristics of the title quaternary salts were studied in H₂O, anhydrous
MeCN, and aqueous EtOH. In the last solvent, 1 of the polarog. waves
gradually disappears. The probable course of the investigated electrode
processes and accompanying chemical transformations is discussed.

ST polarog redn benzyl carbamoylpyridinium chloride; quaternary nicotinamide chloride polarog redn
 IT Substituent effect
 (in polarog. reduction of benzylcarbamoylpyridinium chlorides)
 IT Reduction, electrochemical
 (of benzylcarbamoylpyridinium chloride p-substituted derivs.)
 IT 1652-58-0 5096-13-9 6621-73-4 6951-52-6 52354-19-5
 63828-55-7 84354-35-8 84389-20-8 84389-21-9
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reduction of, electrochem.)
 IT 63828-55-7
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reduction of, electrochem.)
 RN 63828-55-7 HCAPLUS
 CN Pyridinium, 3-(aminocarbonyl)-1-[(4-methoxyphenyl)methyl]-, chloride (9CI)
 (CA INDEX NAME)



● Cl⁻

L57 ANSWER 10 OF 11 HCAPLUS COPYRIGHT 2004 ACS on STN
 AN 1977:480366 HCAPLUS
 DN 87:80366
 ED Entered STN: 12 May 1984
 TI Model dehydrogenase reactions. Catalysis of dihydronicotinamide reductions by noncovalent interactions
 AU Hajdu, Joseph; Sigman, David S.
 CS Sch. Med., Univ. California, Los Angeles, CA, USA
 SO Biochemistry (1977), 16(13), 2841-6
 CODEN: BICHAW; ISSN: 0006-2960
 DT Journal
 LA English
 CC 7-4 (Enzymes)
 AB Carboxylate, pyrophosphate, and hydroxyl groups can accelerate the nonenzymic rates of dihydronicotinamide redns. via intramol. noncovalent interactions. The accelerations by the neg. charged carboxylate and pyrophosphate groups occur in nonpolar solvents but the effect of the hydroxyl groups occurs both in aqueous and nonaq. solution. The largest effects are observed for neighboring carboxylate groups in nonpolar solvents; e.g., the 2nd-order rate constant for the reduction of N-methylacridinium ion by N-cis-2'-carboxycyclopentyl dihydronicotinamide in acetonitrile is 1000-fold more rapid than the rate constant for the corresponding Me ester.

Apparently, the neg. charged carboxylate stabilizes the partial pos. charge which develops on the nicotinamide moiety in the transition state. The conclusion that the neg. charged pyrophosphate can enhance dihydronicotinamide redns. is based on the observation that β -NADH reduces N-methylacridinium ion 30-fold faster in MeOH than in aqueous solution, whereas α -NADH reduces the oxidant only 7-fold faster in MeOH than in water. The pyrophosphate group enhances the reaction rates of both anomers by a distance-dependent field effect. The magnitude is greater for the β anomer because the pyrophosphate and nicotinamide moieties are nearer neighbors in this anomer. The rate accelerations produced by hydroxyl groups of alcs. are not as great as those observed for carboxylate groups in nonpolar solvents. In aqueous solns., α -NADH reduces 3 different oxidants 10-fold more rapidly than β -NADH. In acetonitrile, synthetic dihydronicotinamides containing hydroxyl groups increase the rate 6-fold. These modest accelerations with the neutral hydroxyl groups emphasize the importance of a neg. charged group in order to achieve large enhancements in nonaq. solns.

ST dehydrogenase model dihydronicotinamide redn

IT Functional groups

(diphosphate, in dihydronicotinamide reduction of methylacridinium, dehydrogenase reaction mechanism in relation to)

IT Carboxyl group

Hydroxyl group

(in dihydronicotinamide reduction of methylacridinium, dehydrogenase reaction mechanism in relation to)

IT Kinetics of reduction

(of methylacridinium, by alkyl dihydronicotinamide derivs.)

IT 58-68-4D, analogs 21104-13-2 56133-27-8 56133-28-9 56133-30-3

56133-31-4 56133-32-5 56133-33-6 63761-81-9 63761-82-0

63761-83-1 63761-84-2 63761-85-3 63761-86-4 63761-87-5

63761-88-6 63762-01-6 63762-02-7

RL: RCT (Reactant); RACT (Reactant or reagent)

(N-methylacridinium reduction by, dehydrogenase reaction mechanism in relation to)

IT 17750-24-2

RL: PRP (Properties)

(UV spectra of, solvent effect on)

IT 63762-03-8

RL: RCT (Reactant); RACT (Reactant or reagent)

(chloranil reduction by, dehydrogenase reaction mechanism in relation to)

IT 9035-82-9

RL: PRP (Properties)

(models for, N-alkyl dihydronicotinamide as)

IT 5096-13-9P 7597-54-8P 63761-89-7P 63761-90-0P 63761-91-1P

63761-92-2P 63761-93-3P 63761-94-4P 63761-95-5P 63761-96-6P

63761-97-7P 63761-98-8P 63761-99-9P 63762-00-5P 63828-55-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reduction of)

IT 118-75-2, reactions 13367-81-2

RL: RCT (Reactant); RACT (Reactant or reagent)

(reduction of, by dihydronicotinamide alkyl derivs., dehydrogenase reaction mechanism in relation to)

IT 63828-55-7P

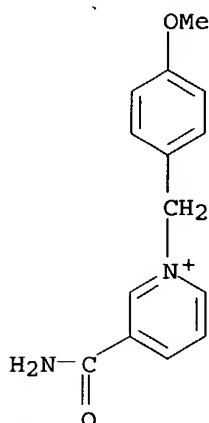
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reduction of)

RN 63828-55-7 HCAPLUS

CN Pyridinium, 3-(aminocarbonyl)-1-[(4-methoxyphenyl)methyl]-, chloride (9CI)

(CA INDEX NAME)



● Cl⁻

- L57 ANSWER 11 OF 11 HCAPLUS COPYRIGHT 2004 ACS on STN
 AN 1963:454780 HCAPLUS
 DN 59:54780
 OREF 59:9970a-c
 ED Entered STN: 22 Apr 2001
 TI Action of base on quaternary salts of nicotinamide
 AU Dittmer, Donald C.; Kolyer, J. M.
 CS Univ. of Pennsylvania, Philadelphia
 SO Journal of Organic Chemistry (1963), 28(9), 2288-94
 CODEN: JOCEAH; ISSN: 0022-3263
 DT Journal
 LA Unavailable
 CC 37 (Heterocyclic Compounds (One Hetero Atom))
 GI For diagram(s), see printed CA Issue.
 AB Treatment of 1benzyl-3-carbamoylpyridinium chloride with NaOH in dilute EtOH yielded a new substance (I), believed to be a cyclic trimer. The structure of I was based on its analysis, infrared spectrum, ultraviolet spectrum, fluorescence spectrum, proton magnetic resonance spectrum, mol. weight, and its chemical reactions. I is believed to have been formed by way of a pyridinium ylide. Several new pseudo base ethers of 1-substituted nicotinamide salts have been prepared
 IT Spectra, visible and ultraviolet
 (of 1,6,11-triazatetracyclo[11.2.2.23.6.28.11]-heneicosa-4,9,14,16,18,20-hexaene-4,9,14-tricarboxamide derivs.)
 IT Spectra, infrared
 (of 1,6,11-triazatetracyclo[11.2.2.23.6.28.11]heneicosa-4,9,14,16,18,20-hexaene-4,9,14-tricarboxamide derivs.)
 IT Nuclear magnetic resonance
 (of 1,6,11-triazatetracyclo[11.2.2.23.6.28.11]heneicosa-4,9,14,16,18,20-hexaene-4,9,14-tricarboxamide derivs.)
 IT Bases
 (reactions of, with 3-carbamoylpyridinium derivs.)
 IT Nitron, α -benzyl-N-[p-(dimethylamino)phenyl]- α -phenyl-Pyridinium, 1-(p-bromobenzyl)-3-carbamoyl-, chloride
 Pyridinium, 1-benzyl-3-carbamoyl-, oxalate
 Pyridinium, 1-benzyl-3-carbamoyl-, picrate
 Pyridinium, 3-carbamoyl-1-(2,4-dinitrobenzyl)-, chloride
 Pyridinium, 3-carbamoyl-1-(p-methoxybenzyl)-, chloride

Pyridinium, 3-carbamoyl-1-(p-nitrobenzyl)-, chloride
 IT Pyridinium, 3-carbamoyl-
 (derivs., reaction with bases)
 IT 952-92-1, Nicotinamide, 1-benzyl-1,4-dihydro- 1652-58-0, Pyridinium,
 3-carbamoyl-1-(p-fluorobenzyl)-, chloride 1893-57-8, Nicotinamide,
 1-(p-fluorobenzyl)-1,4-dihydro- 2996-08-9, Nicotinamide,
 4,4'-oxybis[1-(p-fluorobenzyl)-1,4-dihydro- 4533-64-6,
 1,6,11-Triazatetracyclo[11.2.2.23,6.28,11]heneicosa-4,9,14,16,18,20-
 hexaene-4,9,14-tricarboxamide, 2,7,12-tris(p-fluorophenyl)- 5096-13-9,
 Pyridinium, 1-benzyl-3-carbamoyl-, chloride 6951-52-6, Pyridinium,
 3-carbamoyl-1-(p-chlorobenzyl)-, chloride 13502-54-0, Nicotinamide,
 1-(2,6-dichlorobenzyl)-1,4-dihydro- 19355-18-1, Nicotinamide,
 1-(2,6-dichlorobenzyl)-1,6-dihydro- 75340-29-3, Nicotinamide,
 4,4'-oxybis[1-benzyl-1,4-dihydro- 92578-90-0, Glycine,
 N-(p-tolylsulfonyl)-, 2-(p-bromophenyl)hydrazide 93807-08-0, Glycine,
 N-(phenylsulfonyl)-, 2-(p-bromophenyl)hydrazide 93946-35-1, Glycine,
 N-(p-tolylsulfonyl)-, 2-(m-bromophenyl)hydrazide 94379-06-3,
 Nipicotamide, 1-benzyl-, picrate 95945-13-4, Nicotinamide,
 4,4'-oxybis[1,4-dihydro-1-(p-nitrobenzyl)- 96003-72-4, Nicotinamide,
 4,4'-oxybis[1-(2,6-dichlorobenzyl)-1,4-dihydro- 96635-71-1,
 Nipicotamide, 1-benzyl-, hydrochloride 106141-61-1, 1,6,11-
 Triazatetracyclo[11.2.2.23,6.28,11]heneicosa-4,9,14,16,18,20-hexaene-
 4,9,14-tricarboxamide, 2,7,12-tris(p-bromophenyl)- 106141-62-2,
 1,6,11-Triazatetracyclo[11.2.2.23,6.28,11]heneicosa-4,9,14,16,18,20-
 hexaene-4,9,14-tricarboxamide, 2,7,12-tris(p-chlorophenyl)- 106141-68-8,
 1,6,11-Triazatetracyclo[11.2.2.23,6.28,11]heneicosa-4,9,14,16,18,20-
 hexaene-4,9,14-tricarboxamide, 2,7,12-triphenyl-
 (preparation of)

=> fil uspatall

FILE 'USPATFULL' ENTERED AT 16:11:32 ON 23 JUN 2004

CA INDEXING COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

FILE 'USPAT2' ENTERED AT 16:11:32 ON 23 JUN 2004

CA INDEXING COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

=> d bib abs hitstr tot 156

L56 ANSWER 1 OF 4 USPATFULL on STN

AN 2004:127511 USPATFULL

TI Method for treating fibrotic diseases or other indications IIIC

IN Wagle, Dilip, New York, NY, UNITED STATES

Gall, Martin, Morristown, NJ, UNITED STATES

Bell, Stanley C., Narberth, PA, UNITED STATES

LaVoie, Edmond J., Princeton Junction, NJ, UNITED STATES

PI US 2004097495 A1 20040520

AI US 2003-691839 A1 20031023 (10)

RLI Continuation of Ser. No. US 2001-36857, filed on 31 Dec 2001, PENDING

PRAI US 2000-259294P 20001229 (60)

US 2001-259238P 20010102 (60)

US 2001-296246P 20010606 (60)

DT Utility

FS APPLICATION

LREP MINTZ, LEVIN, COHN, FERRIS, GLOVSKY, AND POPEO, P.C., ONE FINANCIAL
 CENTER, BOSTON, MA, 02111

CLMN Number of Claims: 49

ECL Exemplary Claim: 1

DRWN No Drawings

LN.CNT 3287

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB Provided is a method of treating or ameliorating certain fibrotic
 diseases or other indications in an animal, including a human,

comprising administering an effective amount of a compound of the formula I:

Y--Ar.sup..sym..X.sup.-

wherein Ar.sup..sym. is heteroaryl with a quaternary nitrogen, Y defines certain substitutions on the quaternary nitrogen, and X.sup.- is anion.

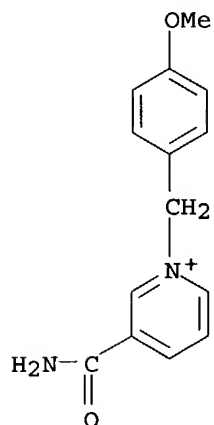
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 63828-55-7P

(preparation of thiadiazolium, pyridinium and pyrimidinium salts for treating fibrotic diseases)

RN 63828-55-7 USPATFULL

CN Pyridinium, 3-(aminocarbonyl)-1-[(4-methoxyphenyl)methyl]-, chloride (9CI)
(CA INDEX NAME)



● Cl⁻

L56 ANSWER 2 OF 4 USPATFULL on STN

AN 2003:30319 USPATFULL

TI Novel agents for replacement of NAD⁺/NADH system in enzymatic reactions

IN Fish, Richard H., Berkeley, CA, UNITED STATES

Kerr, John B., Oakland, CA, UNITED STATES

Lo, Christine H., Solana Beach, CA, UNITED STATES

PI US 2003022266 A1 20030130

US 6716596 B2 20040406

AI US 2001-805726 A1 20010312 (9)

DT Utility

FS APPLICATION

LREP Hana Verny, Peters, Verny, Jones & Biksa LLP, 385 Sherman Avenue, Suite 6, Palo Alto, CA, 94306

CLMN Number of Claims: 18

ECL Exemplary Claim: 1

DRWN 8 Drawing Page(s)

LN.CNT 1777

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB Novel agents acting as co-factors for replacement of NAD(P).sup.+/NAD(P)H co-enzyme systems in enzymatic oxido-reductive reactions. Agents mimicking the action of NAD(P).sup.+/NAD(P)H system in enzymatic oxidation/reduction of substrates into reduced or oxidized products. A method for selection and preparation of the mimicking agents

for replacement of NAD(P).sup.+ / NAD(P)H system and a device comprising
co-factors for replacement of NAD(P).sup.+ / NAD(P)H system.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 459165-10-7P

(NAD(P) mimic for use in enzymic redox reactions)

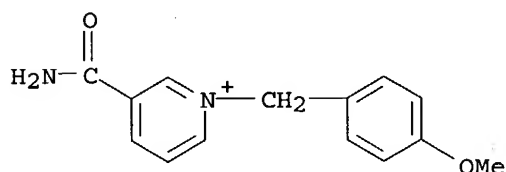
RN 459165-10-7 USPATFULL

CN Pyridinium, 3-(aminocarbonyl)-1-[(4-methoxyphenyl)methyl]-, salt with
trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 175979-55-2

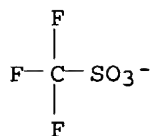
CMF C14 H15 N2 O2



CM 2

CRN 37181-39-8

CMF C F3 O3 S



L56 ANSWER 3 OF 4 USPATFULL on STN

AN 2002:323196 USPATFULL

TI Method for treating fibrotic diseases or other indications IIIC

IN Wagle, Dilip, New York, NY, UNITED STATES

Gall, Martin, Morristown, NJ, UNITED STATES

Bell, Stanley C., Narberth, PA, UNITED STATES

LaVoie, Edmond J., Princeton Junction, NJ, UNITED STATES

PI US 2002183365 A1 20021205

AI US 2001-36857 A1 20011231 (10)

PRAI US 2001-296246P 20010606 (60)

US 2001-259238P 20010102 (60)

US 2000-259294P 20001229 (60)

DT Utility

FS APPLICATION

LREP ALLEN BLOOM, C/O DECHERT, PRINCETON PIKE CORPORATION CENTER, P.O. BOX
5218, PRINCETON, NJ, 08543-5218

CLMN Number of Claims: 49

ECL Exemplary Claim: 1

DRWN No Drawings

LN.CNT 3334

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB Provided is a method of treating or ameliorating certain fibrotic
diseases or other indications in an animal, including a human,
comprising administering an effective amount of a compound of the

formula I:

Y--Ar.sym..multidot.X.sup.--

wherein:

a. Ar is a five or six membered heteroaryl ring having a first ring nitrogen and optionally second or third ring nitrogens, with the remaining ring atoms being carbon, oxygen, or sulfur, provided the first nitrogen of Ar is a quaternary nitrogen and Ar is not thiazolium, oxazolium or imidazolium;

b. Y is substituted on the first ring nitrogen, with the proviso that if Ar is pyrazole, indazole, (1,2,3)-triazole, benzotriazole, or (1,2,4)-triazole, the second ring nitrogen is substituted

c. Y is:

1. a group of the formula --CH(R.sup.5)--R.sup.6 [as preferred in one embodiment]

(a) wherein R.sup.5 is hydrogen, alkyl, cycloalkyl-, alkenyl-, alkynyl-, aminoalkyl-, hydroxy[C.sub.1 to C.sub.6]alkyl, dialkylaminoalkyl-, (N-[C.sub.6 or C.sub.10]aryl)(N-alkyl)aminoalkyl-, piperidin-1-ylalkyl-, pyrrolidin-1-ylalkyl, azetidinyllalkyl, 4-alkylpiperazin-1-ylalkyl, 4-alkylpiperidin-1-ylalkyl, 4-[C.sub.6 or C.sub.10]arylpiperazin-1-ylalkyl, 4-[C.sub.6 or C.sub.10]arylpiperidin-1-ylalkyl, azetidin-1-ylalkyl, morpholin-4-ylalkyl, thiomorpholin-4-ylalkyl, piperazin-1-ylalkyl, piperidin-1-ylalkyl, [C.sub.6 or C.sub.10]aryl, or independently the same as R.sup.6;

(b) wherein R.sup.6 is

(1) hydrogen, alkyl (which may be substituted by alkoxy carbonyl)-, alkenyl, alkynyl, cyano-, cyanoalkyl-, or Rs, wherein Rs is a [C.sub.6 or C.sub.10]aryl or a heterocycle containing 4-10 ring atoms of which 1-3 are heteroatoms selected from the group consisting of oxygen, nitrogen and sulfur; or

(2) a group of the formula --W--R.sup.7 [as preferred in one embodiment], wherein R.sup.7 is alkyl, alkoxy, hydroxy, or Rs [as preferred in one embodiment], wherein W is --C(.dbd.O)-- or --S(O).sub.2--;

(3) a group of the formula --W--OR.sup.8 wherein R.sup.8 is hydrogen or alkyl,

(4) a group of the formula --CH(OH)Rs; or

(5) a group of the formula --W--N(R.sup.9)R.sup.10, wherein

(a) R.sup.9 is hydrogen and R.sup.10 is an alkyl or cycloalkyl, optionally substituted; or

(b) R.sup.9 is hydrogen or alkyl and R.sup.10 is Ar; or

(c) R.sup.9 is hydrogen or alkyl, R.sup.10 is a heterocycle containing 4-10 ring atoms of which 1-3 are heteroatoms are selected from the group consisting of oxygen, nitrogen and sulfur; or

(d) R.sup.9 and R.sup.10 are both alkyl groups; or

(e) R.sup.9 and R.sup.10 together with N form a heterocycle containing

4-10 ring atoms which can incorporate up to one additional heteroatom selected from the group of N, O or S in the ring, wherein the heterocycle is optionally substituted; or

(f) R.sup.9 and R.sup.10 are both hydrogen; or

2. --NH.sub.2, and

e. X is a pharmaceutically acceptable anion, which may be absent if the compound provides a neutralizing salt, or

(B) a pharmaceutically acceptable salt of the compound.

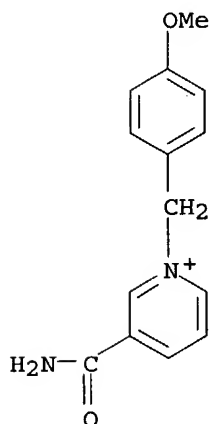
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 63828-55-7P

(preparation of thiadiazolium, pyridinium and pyrimidinium salts for treating fibrotic diseases)

RN 63828-55-7 USPATFULL

CN Pyridinium, 3-(aminocarbonyl)-1-[(4-methoxyphenyl)methyl]-, chloride (9CI)
(CA INDEX NAME)



● Cl⁻

L56 ANSWER 4 OF 4 USPAT2 on STN

AN 2003:30319 USPAT2

TI Agents for replacement of NAD⁺/NADH system in enzymatic reactions

IN Fish, Richard H., Berkeley, CA, United States

Kerr, John B., Oakland, CA, United States

Lo, Christine H., Solana Beach, CA, United States

PA The Regents of the University of California, Oakland, CA, United States
(U.S. corporation)

PI US 6716596 B2 20040406

AI US 2001-805726 20010312 (9)

DT Utility

FS GRANTED

EXNAM Primary Examiner: Gitomer, Ralph

LREP VERNY, HANA

CLMN Number of Claims: 18

ECL Exemplary Claim: 1

DRWN 12 Drawing Figure(s); 7 Drawing Page(s)

LN.CNT 1759

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB . Novel agents acting as co-factors for replacement of NAD(P).sup.+/NAD(P)H co-enzyme systems in enzymatic oxido-reductive reactions. Agents mimicking the action of NAD(P).sup.+/NAD(P)H system in enzymatic oxidation/reduction of substrates into reduced or oxidized products. A method for selection and preparation of the mimicking agents for replacement of NAD(P).sup.+/NAD(P)H system and a device comprising co-factors for replacement of NAD(P).sup.+/NAD(P)H system.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 459165-10-7P

(NAD(P) mimic for use in enzymic redox reactions)

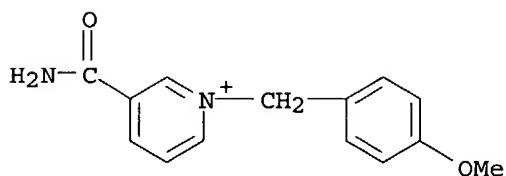
RN 459165-10-7 USPAT2

CN Pyridinium, 3-(aminocarbonyl)-1-[(4-methoxyphenyl)methyl]-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 175979-55-2

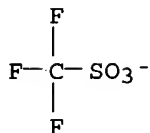
CMF C14 H15 N2 O2



CM 2

CRN 37181-39-8

CMF C F3 O3 S



=>